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Charge Transfer Complexes: N_4^+, N_2CO^+ and $OCCO^+$

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In the dense region of planetary ionospheres, the charge transfer complexes N_4^+ [1], N_2CO^+ [2] and $OCCO^+$ play an important role as intermediates in the collisional energy redistribution in the diatomic fragments. Using electronic structure calculations six-dimensional potential energy functions have been generated for the electronic ground states, and one-dimensional collinear cuts for the central bond stretching coordinate in the excited states.

In the case of N_4^+ and N_2CO^+ six-dimensional variational calculations have been employed to calculate anharmonic vibrational levels for energies up to about 3000 cm^{-1} in the $^2\Sigma_u^+$ (N_4^+) or A' (N_2CO^+) electronic ground states. Apart from the two stretching modes related to the diatoms all others modes exhibit large amplitudes due to the quasi van der Waals character of the corresponding potential energy regions.

It is shown that in all three ions the first electronically excited states are $^2\Pi$ states with much smaller central bond distances than in the ground states. In the electronically excited states several conical intersections have been found.

[1] C. Léonard, P. Rosmus, S. Carter and N.C. Handy, J. Phys. Chem. A, **103**, 1846 (1999).

[2] M. Hochlaf, C. Léonard, E.E. Ferguson, P. Rosmus, E.-A. Reinsch, S. Carter and N.C. Handy, J. Chem. Phys., **111**, 4948 (1999).